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Numerical Simulations on Szilard's Engine and Information Erasure

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Abstract

We present a computational model for Szilard's engine and the information discarding process. Taking advantage of a fact that the one is essentially the reversed cycle of the other, we can discuss the both by employing the same model. Through numerical simulations we calculate the work extracted by the engine and the heat generation in the information discarding process. It is found that these quantities depend on some realistic ingredients, which means that the work done by the engine is no longer canceled by the heat generation in the information erasure.

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In 1876, Maxwell invented an external agent which utilizes information to extract the work from a single heat bath as a perpetual cycle [1]. It is now known as Maxwell's demon. One of the simplest configurations related to Maxwell's demon was presented by Szilard [2]. It consists of one molecule captured in a cylinder in contact with a heat bath. The demon inserts the piston in the middle of the cylinder, observes which side the molecule is in, and then expand it to extract the work from the heat bath. After the expansion, the demon removes the piston and repeats the same manipulation. Based on some assumptions, Szilard showed that the work of $k_B T \log 2$ can be extracted per one cycle. This cycle seems to violate the second law of thermodynamics and has provoked many arguments among physicists since presented [3].

Most of the physicists sought heat generation outside of the engine. In particular Brillouin [4] studied concrete measurement processes and attempted to prove that such measurements should be accompanied by heat generation. Although his argument is attractive, one can always counterargue that there may be another measurement process without heat generation. Indeed Bennett suggested that reversible measurements are possible and proposed a new interpretation for the Maxwell's demon problem [5]. His argument is as follows. For the total system to be a complete cycle, the information of the preceding cycle stored in the manipulator must be discarded before succeeding cycles. Following to the Landauer's claim, logically irreversible processes such as information erasure should be accompanied by heat generation at least $k_B T \log 2$ per bit [6]. It might be plausible that the extracted work of $k_B T \log 2$ by utilizing 1-bit information is compensated by heat generation of 1-bit information erasure. Owing to their cancelation, the total system is expected to be consistent with the second law.

While the above argument seems reasonable, we have some doubts about the evaluation of the extracted work by the engine and generated heat in memory erasure, because the thermodynamic nature of the information might depend on its physical embodiment. Especially the discussions so far are confined to idealized situation by means of thought experiments. In this Letter, we study energetics of computational models for Szilard's engine and information erasure by taking some realistic components into account.

First, we present a computational model for Szilard's engine. Our model is one dimensional so that we can describe this system by a velocity and a position of the piston V, X and ones of the particle v, x. (See Fig. 1.) Let the mass of the particle and the piston be m and M, respectively. The position of the particle is restricted to the region $-L < x < L$, where L is the half length of the cylinder. We assume evolution equations for X and x as

$$M\frac{dV}{dt} = -\frac{\partial U(X,t)}{\partial X} - \zeta V + \xi(t) + f(t), \tag{1}$$

$$m\frac{dv}{dt} = -f(t) - g(t), \tag{2}$$

where $\xi(t)$ is Gaussian white noise whose statistical properties are characterized by $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\xi(t') \rangle = 2\zeta k_B T \delta(t-t')$. $g(t)$ and $f(t)$ are the momentum transfer per unit time from the particle to the heat bath and to the piston, respectively.

$g(t)$ is given implicitly by a stochastic rule at the boundaries $x = \pm L$ in such a way that the particle is reflected being assigned new velocity v at random with the probability distribution function

$$\phi(v) = \frac{m|v|}{k_B T}\exp[-\frac{mv^2}{2k_B T}]. \tag{3}$$

The distribution of the particle velocity turns out to be Maxwellian when there is only a single particle in the system [7]. Note that the piston is assumed not to undergo the reflection at the boundary.

The form of $f(t)$ is given on the assumption that the piston and the particle collide elastically. After a collision of the particle and the piston, they become

$$V' = \frac{1-\epsilon}{1+\epsilon}V + \frac{2\epsilon}{1+\epsilon}v, \tag{4}$$

$$v' = \frac{2}{1+\epsilon}V - \frac{1-\epsilon}{1+\epsilon}v, \tag{5}$$

where $\epsilon \equiv m/M$. Since the momentum transfer from the particle to the piston is $2m(v-V)/(1+\epsilon)$, we obtain

$$f(t) = \sum_i \frac{2m}{1+\epsilon}(v-V)\delta(t-t_i), \tag{6}$$

where $\delta(t)$ denotes Dirac's delta function and t_i represents the time when i-th collision takes place.

The demon manipulates the piston through a trapping potential $U(x,t)$. We assume the form of the potential as

$$U(X,t) = \frac{k}{2}(X - X_0(t))^2. \tag{7}$$

The form of $X_0(t)$ is given as the demon's manipulation. In this paper, we assume

$$X_0(t) = \begin{cases} \pm lt/\tau & (0 \le t \le \tau) \\ \pm l(2 - t/\tau) & (\tau \le t \le 2\tau), \end{cases} \tag{8}$$

where the choice of the sign in the time interval $0 \le t \le \tau$ depends on the relative position of the particle to the piston. (The sign is positive for $X > x$, while negative for $x < X$.) The sign of $X_0(t)$ during $\tau \le t \le 2\tau$ is determined so that $X_0(t)$ becomes continuous. Further, the piston is assumed to be removed at $t = \tau$ and to be reinserted at $t = 2\tau$. $f(t)$ becomes zero during $\tau \le t \le 2\tau$, which means that the piston is outside of the cylinder. In this way, the demon can repeat cycles. The manipulation by the demon is shown in Fig. 2.

Note that l can be larger value than L, because the piston can collide with the particle even if $|X_0(t)| > L$. Yet, since the difference of physical quantities such as work and heat between $l = L$ and $l > L$ is expected to be negligible when k is large enough to localize the piston, hereafter we let $l = L$.

Next we present a computational model for a memory erasing process. We first notice that such a process can be designed as the reversed one of a Szilard's cycle. Initially, the piston is assumed to be in the middle of the cylinder. The particle is confined in one side (left or right) of it, which encodes an informational bit. After the piston is removed, it is reinserted in the left end of the cylinder and moved to the middle. The particle is now in

the right side. This operation turns out to be the reversed one of a Szilard's cycle as shown in Fig. 3, and to be a logically irreversible process to discard the information at the initial state (left or right) as shown in Fig .4. Since we already have a computational model for Szilard cycles, we can easily realize the reversed Szilard cycle by employing the above model given by Eqs. (1) and (2). All assumptions are the same except for the manipulation of the piston such that

$$X_0(t) = \begin{cases} -Lt/\tau & (0 \le t \le \tau) \\ L(t/\tau - 2) & (\tau \le t \le 2\tau). \end{cases} \tag{9}$$

We also note that $f(t) = 0$ when $0 \le t \le \tau$.

We now discuss the energetics of our model. We first assume that the removement and the reinsertion of the piston cost no energy. The validity of this assumption can be proved by analyzing a suitable model for this process [9]. On this assumption, we study the energetics of Eqs. (1) and (2). We follow the energetic interpretation for Langevin equations, which has been proposed by Sekimoto recently [8]. By multiplying Eqs. (1) and (2) by $V(t)dt$ and $v(t)dt$ respectively and integrating over one cycle, we obtain

$$\begin{aligned} &\int_0^{2\tau} MV(t)dV(t) + \int_0^{2\tau} \frac{\partial U(X,t)}{\partial X} V(t)dt \\ &= \int_0^{2\tau} (-\zeta V(t) + \xi(t) + f(t))V(t)dt, \end{aligned} \tag{10}$$

$$\int_0^{2\tau} mv(t)dv(t) = -\int_0^{\tau} f(t)v(t)dt + \int_0^{2\tau} g(t)v(t)dt. \tag{11}$$

These integrals are assumed as Stratonovich calculus for the following discussions being valid. We analyze Eq.(10) first. The first term of the left-handed side is written as the kinetic energy difference denoted by $\Delta K \equiv \Delta MV^2/2$. We can rewrite the second term as

$$\int dU - \int \frac{\partial U(X,t)}{\partial t} dt \equiv \Delta U + W, \tag{12}$$

where W is defined as

$$W \equiv -\int_0^{2\tau} \frac{\partial U(X,t)}{\partial t} dt, \tag{13}$$

which corresponds to the work done by the engine.

The first two terms of the right-handed side of Eq. (10) is denoted by $-Q_1$, where Q_1 is interpreted to be the energy dissipation to the heat bath. The last term then corresponds to the energy gain from the particle, which is denoted by C, that is,

$$C \equiv \int_0^{2\tau} f(t)V(t)dt. \tag{14}$$

Then, Eq. (10) becomes

$$\Delta K + \Delta U + W = -Q_1 + C. \tag{15}$$

Similarly, by analyzing Eq. (11) as we did for Eq. (10), we obtain

$$\Delta K' = -C - Q_2, \tag{16}$$

where $Q_2 = -\int g(t)v(t)dt$ is the energy transfer from the particle to the heat bath and $\Delta K'$ is a kinetic energy increase of the particle. The total generated heat Q, the energy transferred from the system to the heat bath, is given by

$$Q = Q_1 + Q_2. \tag{17}$$

Using these notations, we have en energy conservation law

$$\Delta K + \Delta K' + \Delta U + W + Q = 0. \tag{18}$$

Note that this expression holds for each of succeeding cycles. By taking an average over many cycles, we obtain

$$\langle W\rangle + \langle Q\rangle = 0. \tag{19}$$

In the argument below, $\langle\rangle$ denotes the average over many cycles.

Now we are ready to perform numerical simulations. We calculated the time evolution by a second order Runge-Kutta method. We let $k_BT = 1, M = 1$, and $L = 1$ for non-dimensionization and hence dimensionless parameters are ϵ, k, ζ and τ. We are particularly concerned with the ϵ dependence of the work by the engine $\langle W\rangle_e$ and the heat generation in the memory $\langle Q\rangle_m$. In Fig.5, we plotted the result of simulations with the parameter values $\tau = 10$, $k = 100$ and $\zeta = 0.1$. For large ϵ, the work and the heat generation goes below from $k_BT\log 2$. It is also found that we get less work with smaller k. Our simulations suggest that the maximum work $k_BT\log 2$ is obtainable in the limit of $\epsilon \to 0$, $k \to \infty$ and $\tau \to \infty$.

These results show that the compensation does not occur unless we adopt exactly the same ϵ for the engine and the memory. Moreover, total heat absorption in the engine cycle and the memory reset process is possible. Hence the interpretation of Maxwell's demon problem by Bennett and Landauer [5] is not applicable to this model.

Furthermore, owing to the operationally inverse relation between the information erasure and the engine, we define the reversible heat generation $\langle Q\rangle_{rev}$ and irreversible one $\langle Q\rangle_{irr}$ as

$$\langle Q\rangle_{rev} = (\langle Q\rangle_m - \langle Q\rangle_e)/2, \tag{20}$$
$$\langle Q\rangle_{irr} = (\langle Q\rangle_m + \langle Q\rangle_e)/2. \tag{21}$$

In Fig. 6, $\langle Q\rangle_{rev}$ and $\langle Q\rangle_{irr}$ were plotted against τ while fixing the other parameter values as $\epsilon = 10^{-4}$, $\zeta = 1$ and $k = 100$. We found that $\langle Q\rangle_{rev}$ and $\langle Q\rangle_{irr}$ are closed to $k_BT\log 2$ and $2\zeta/\tau$, respectively. When the entropy production is defined through the irreversible heat generation, it becomes zero in the quasi-static limit. Do not confuse this fact with an incorrect statement that the heat generation during information erasure can be zero [10], because the generated heat during logically irreversible processes has a positive reversible part.

Here we address three remarks on our results. First, for generality of our results, we have studied another model where the single particle obeys the following equation instead of Eq. (2),

$$m\frac{dv}{dt} = -\bar{\zeta}\frac{dx}{dt} + \bar{\xi}(t) - f(t), \tag{22}$$

where $\langle \bar{\xi} \rangle = 0$ and $\langle \bar{\xi}(t) d\bar{\xi}(t') \rangle = 2\bar{\zeta} k_B T \delta(t-t')$. We confirmed that this model yields a qualitatively same graph as Fig. 5.

Second, with some purturbative calculations, we get an analytic expression of the work done by the engine

$$\langle W \rangle_e = \frac{1-\epsilon}{1+\epsilon} k_B T \log 2 - \frac{2\zeta}{\tau}, \tag{23}$$

where we have assumed that ϵ is small and $k \to \infty$. Similarly, as to the heat generation in the information erasure process,

$$\langle Q \rangle_m = \frac{1-\epsilon}{1+\epsilon} k_B T \log 2 + \frac{2\zeta}{\tau}. \tag{24}$$

These expressions are good agreement with the results of simulations where $\epsilon < 0.03$.

Finally, we stress here the difference between our discussions and analysis recently presented by Magnasco [11]. His analysis is on the system described by a Fokker-Planck equation and applies to the automatic engine which needs no observer. It was proposed by Popper [12] as an objection to the notion that information is equivalent to negentropy (negative entropy) [4]. While the engine needs no observer (hence no memory), Magnasco showed that it cannot work as a perpetual cycle. His argument does not apply to the problem we discuss, since our system is assumed to be manipulated by the external agent which makes observation.

In conclusion, we invent a concrete model for Szilard's engine. Numerical simulations show that its energy transformation ability from the heat to mechanical work depends on parameters, especially the mass ratio of the particle and the piston. We also find that an information erasure process need not cost $k_B T \log 2$ energy in the same model. As to the Maxwell's demon problem, the work obtained is not canceled with the generated heat in the information discarding process.

The arising question out of our results is on the consistency with the second law. As mentioned above, the interpretation of the Maxwell's demon problem does not hold on the assumptions we adopt, and hence the second law neither. As a plausible answer to the question, we conjecture that the excess heat is generated in the measurement process which transfers information from the engine to the memory. Even if a reversible measurement is possible, it may be realized only for particular devices. (In our case, ϵ of the engine and the memory are precisely the same value.) When the embodiment of the information in the memory part is different from that of the engine part, the excess heat may be necessary in the information transferring process. These are future problems to be considered.

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FIGURES

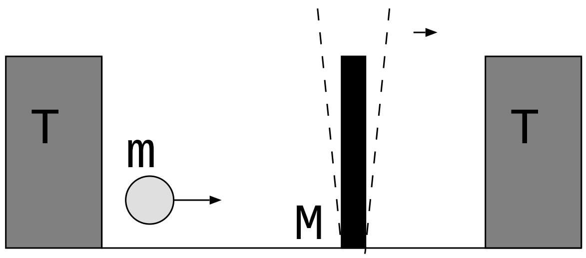


FIG. 1. Schematic figure of our model for Szilard's engine.

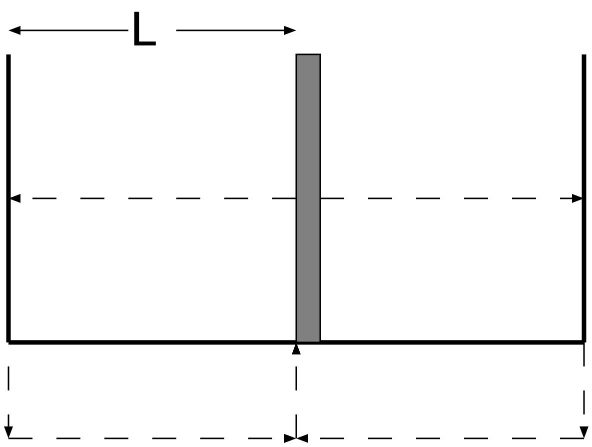


FIG. 2. Demon's manipulation of Szilard's engine.

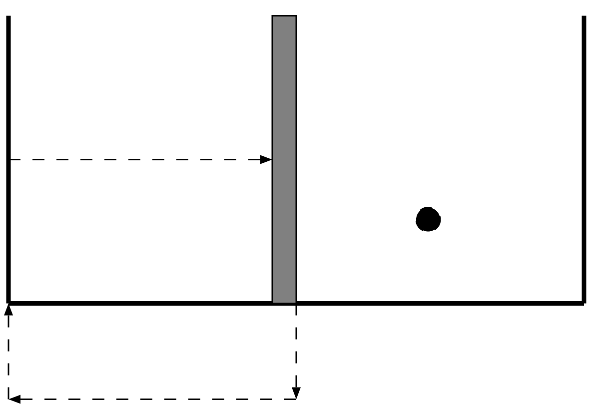


FIG. 3. Reversed operation of Szilard's engine.

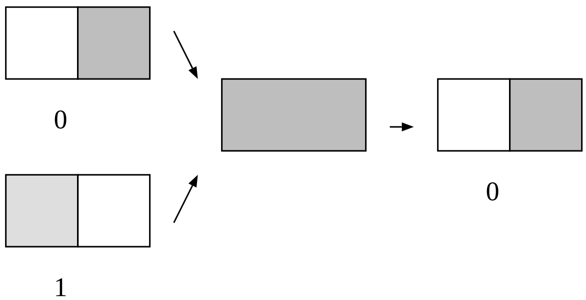


FIG. 4. Schematic figure of information discarding process.

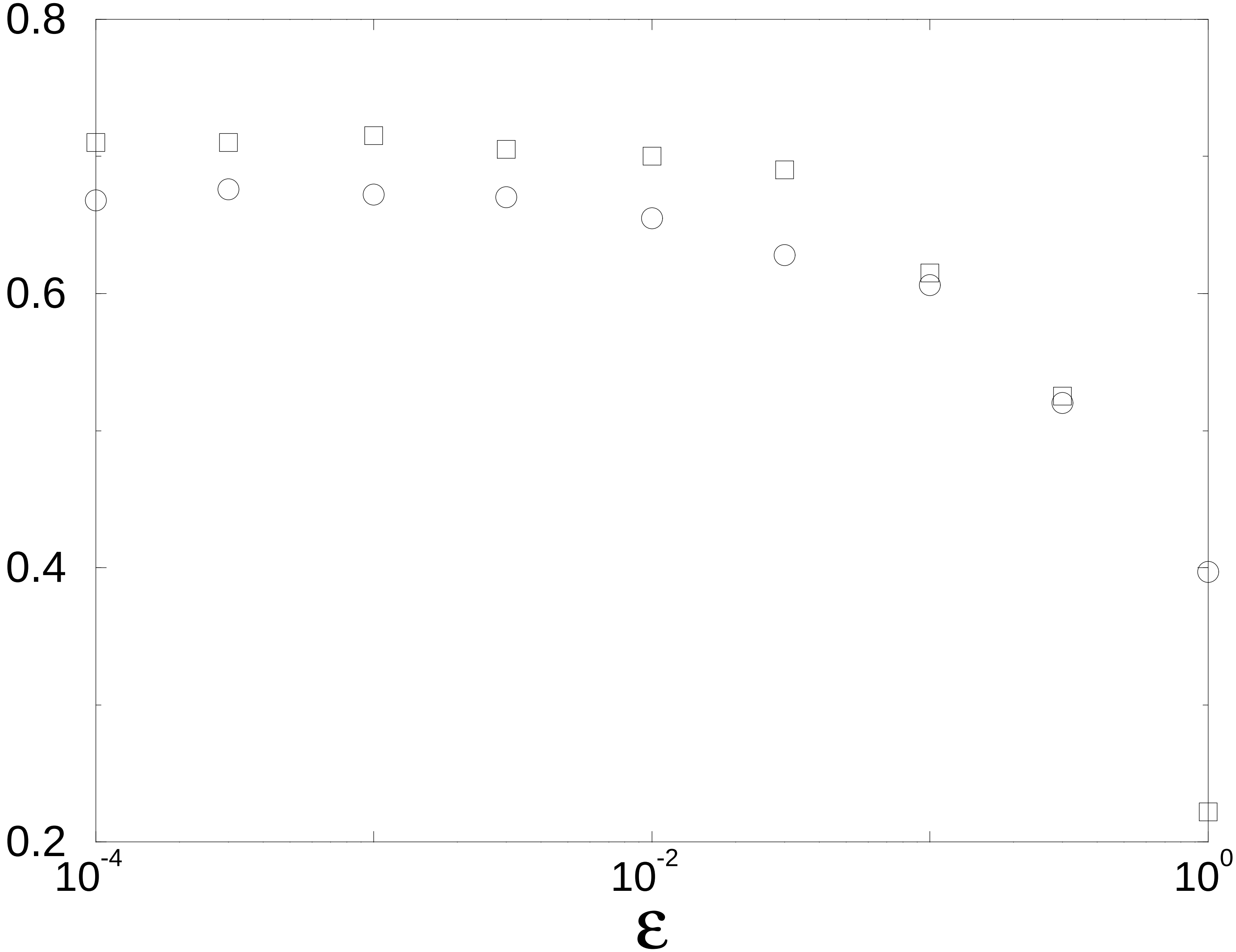
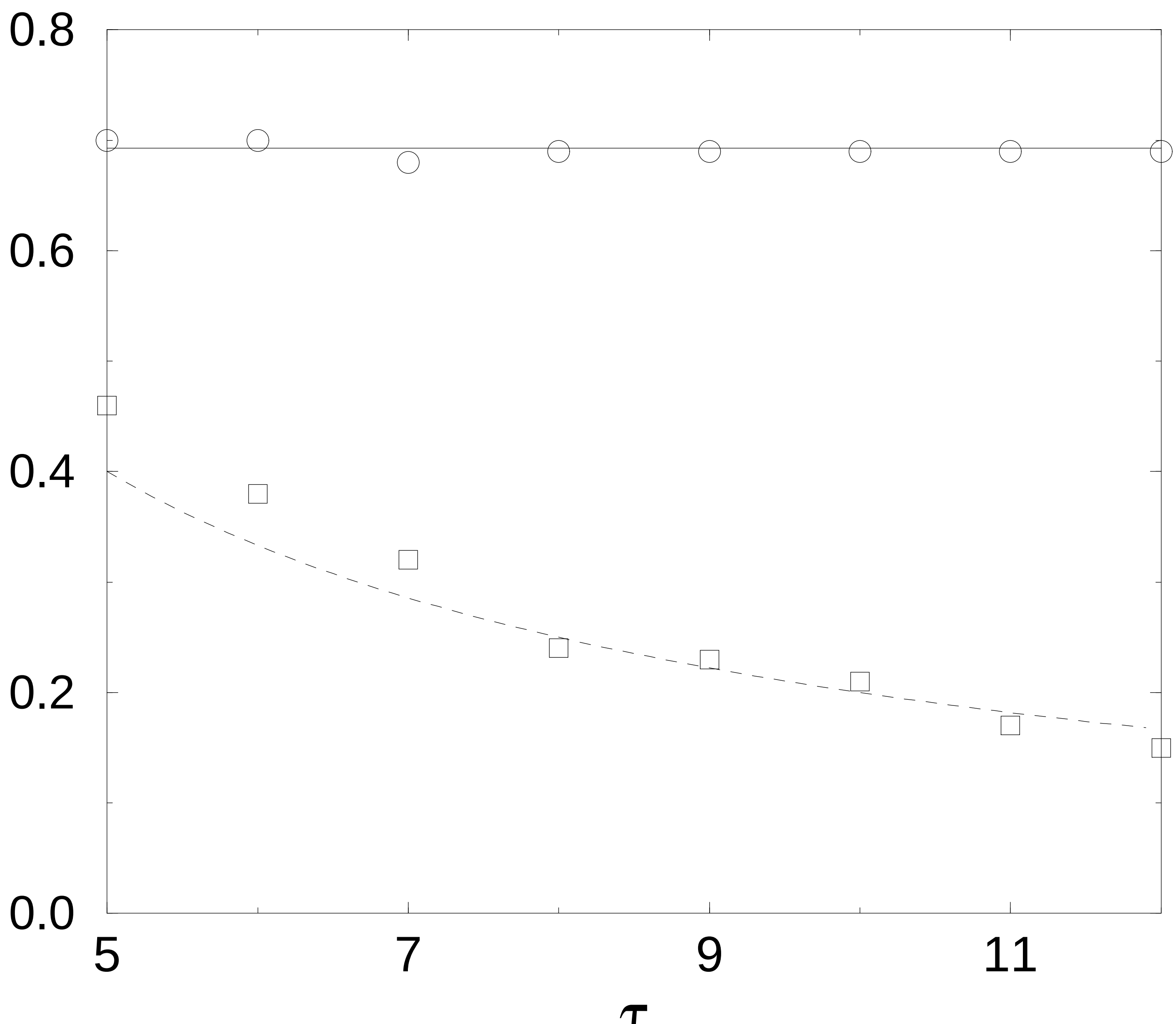

0.8
0.6
0.4
0.2
10^{-4}
10^{-2}
10^{0}
ε

FIG. 5. $\langle W \rangle_e$ (circles) and $\langle Q \rangle_m$ (squares) versus ϵ. These were obtained as averages over 5000 cycles.


0.8
0.6
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0.2
0.0
5
7
9
11

FIG. 6. $\langle Q\rangle_{rev}$ (circles) and $\langle Q\rangle_{irr}$ (squares) versus τ. The solid line is $k_B T \log 2$ and the dotted line is $2\zeta/\tau$.